REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. REPORT DATE *(DD-MM-YYYY)*
November 2014

2. REPORT TYPE
Briefing Charts

3. DATES COVERED *(From - To)*
November 2014- November 2014

4. TITLE AND SUBTITLE
Optimal Numerical Schemes for Time Accurate Compressible Large Eddy Simulations: Comparison of Artificial Dissipation and Filtering Schemes

5a. CONTRACT NUMBER
N/A

5b. GRANT NUMBER

5c. PROGRAM ELEMENT NUMBER

6. AUTHOR(S)
Edoh, A., Karagozian, A., Merkle, C. and Sankaran, V.

5d. PROJECT NUMBER

5e. TASK NUMBER

5f. WORK UNIT NUMBER
Q12J

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
Air Force Research Laboratory (AFMC)
AFRL/RQR
5 Pollux Drive.
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8. PERFORMING ORGANIZATION REPORT NO.

9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES)
Air Force Research Laboratory (AFMC)
AFRL/RQR
5 Pollux Drive.
Edwards AFB CA 93524-7048

10. SPONSOR/MONITOR'S ACRONYM(S)

11. SPONSOR/MONITOR'S REPORT NUMBER(S)
AFRL-RQ-ED-VG-2014-321

12. DISTRIBUTION / AVAILABILITY STATEMENT
Distribution A: Approved for Public Release; Distribution Unlimited.

13. SUPPLEMENTARY NOTES
Briefing Charts presented at 67th American Physical Society (APS) Meeting, San Francisco, CA, 23-25 Nov, 2014. PA#14565

14. ABSTRACT
N/A

15. SUBJECT TERMS

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
					Venke Sankaran
a. REPORT	b. ABSTRACT	c. THIS PAGE	SAR	23	19b. TELEPHONE NO *(include area code)*
Unclassified	**Unclassified**	**Unclassified**			661-275-5634

Standard Form 298 (Rev. 8-98)
Prescribed by ANSI Std. 239.18

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THE AIR FORCE RESEARCH LABORATORY
LEAD | DISCOVER | DEVELOP | DELIVER

Optimal Numerical Schemes for Time Accurate Compressible Large Eddy Simulations:

Comparison of Artificial Dissipation and Filtering Schemes

Ayaboe Edoh, Ann Karagozian (UCLA)
Charles Merkle (Purdue), Venke Sankaran (AFRL)

Research Supported by AFOSR (Drs. Fahroo and Li, PMs)

UCLA ENERGY & PROPULSION RESEARCH LABORATORY

67th American Physical Society (APS) Meeting

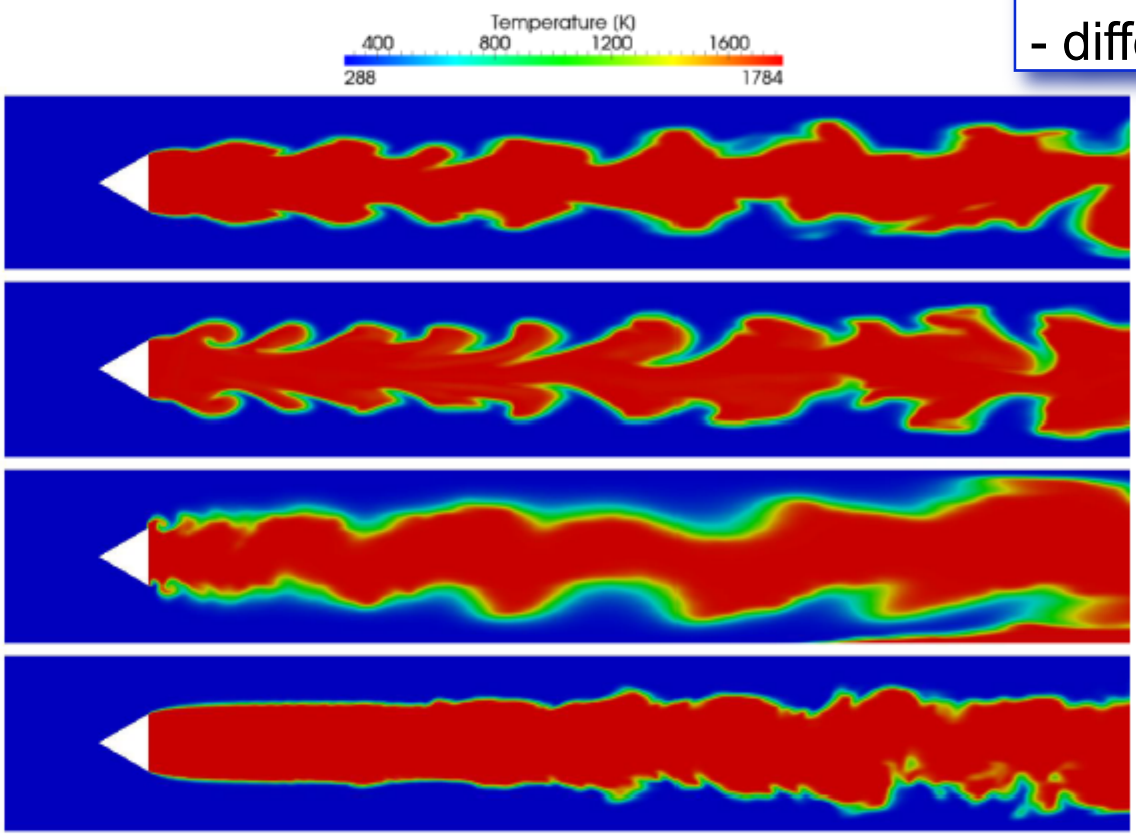
Division of Fluid Dynamics

San Francisco, CA

November 23-25, 2014

Challenges: Reactive LES

Algorithm comparisons:
- identical subgrid modeling
- differences reside in numerics



CHARLES (Stanford)

LESLIE3D (Georgia Tech)

OpenFOAM (OpenCFD)

Fluent (Ansys)

Ref: 2013 - Cocks, Sankaran, Soteriou, "Is LES of reacting flow predictive? Part 1: Impact of Numerics"

Need to determine **BEST** discretization schemes for Reacting LES

Objectives

GOAL:

damp high frequency errors while preserving low wave content (ie: low-pass response)

1) compare damping character of Artificial Dissipation and Filtering

2) formulate filter as an equivalent Artificial Dissipation scheme
   - consequence of filter damping for stiff problems

3) insight on achieving "ideal" low-pass response for general problems

- von Neumann Analysis
- Crank-Nicolson w/ 6^{th} order central differencing

von Neumann Analysis

1D Euler System (quasi-linear form):

$$\frac{\partial Q}{\partial t} + A\frac{\partial Q}{\partial x} = 0$$

$$Q_i = \sum_k \hat{Q}(k)e^{ikx}$$

$$Q_{i+i} = \sum_k \hat{Q}(k)e^{ik(x+\Delta x)} = \sum_k \hat{Q}(k)e^{ik\Delta x}e^{ikx} \qquad k\Delta x = \theta$$

with $\theta \in [-\pi, \pi]$

$$\boxed{Q^{n+1} = G(\theta)Q^n}$$

Eigenvalues of the amplification matrix specify growth factor and phase errors.

Growth Factor

$$\boxed{|g_i|_2}$$

Phase Error

$$\boxed{\frac{\phi}{\phi_{exact}} = \frac{-\tan^{-1}\{\mathrm{Im}(g_i)/\mathrm{Re}(g_i)\}}{CFL_i \times \theta}}$$

Artificial Dissipation

$$\frac{\partial Q}{\partial t} + A\frac{\partial Q}{\partial x} = \sum_m (-1)^{m-1}(\Delta x)^{2m-1}\varepsilon_{2m}\left|\lambda_{u+c}\right|\frac{\partial^{2m}Q}{\partial x^{2m}}$$

governing equations augmented with dissipation terms

$$\varepsilon_2 = 1/2$$
$$\varepsilon_4 = 1/12$$
$$\varepsilon_6 = 1/60$$

upwind biased stencils

m = 1: $$\frac{Q_{i+1}-Q_{i-1}}{2\Delta x} - \frac{1}{2}\left(\frac{Q_{i+1}-2Q_i+Q_{i-1}}{\Delta x}\right) = \frac{Q_i - Q_{i-1}}{\Delta x}$$

m = 2: $$\frac{-Q_{i+2}+8Q_{i+1}-8Q_{i-1}+Q_{i-2}}{12\Delta x} + \frac{1}{12}\left(\frac{Q_{i+2}-4Q_{i+1}+6Q_i-4Q_{i-1}+Q_{i-2}}{\Delta x}\right) = \frac{4Q_{i+1}+6Q_i-12Q_{i-1}+2Q_{i-2}}{12\Delta x}$$

etc…

Filtering (Explicit)

$$Q_i = \left[1 + \sum_m S_{2m} (\Delta x)^{2m} \frac{\partial^{2m}}{\partial x^{2m}} \right] Q_i^*$$

smoothing of solution as post-process of integration step

represent total amplification of filter scheme as:

$$G(\theta) = R(\theta) G^*(\theta)$$

with $\begin{cases} \left| R(\theta) \right|_2 \leq 1 \\ R(\theta = \pm\pi) = 0 \end{cases}$

NOTE: filter is purely dissipative and does not alter original scheme's phase behavior

Filtering (Implicit)

$$\left[1+\sum_m S'_{2m}(\Delta x)^{2m}\frac{\partial^{2m}}{\partial x^{2m}}\right]Q_i=\left[1+\sum_m S_{2m}(\Delta x)^{2m}\frac{\partial^{2m}}{\partial x^{2m}}\right]Q_i^*$$

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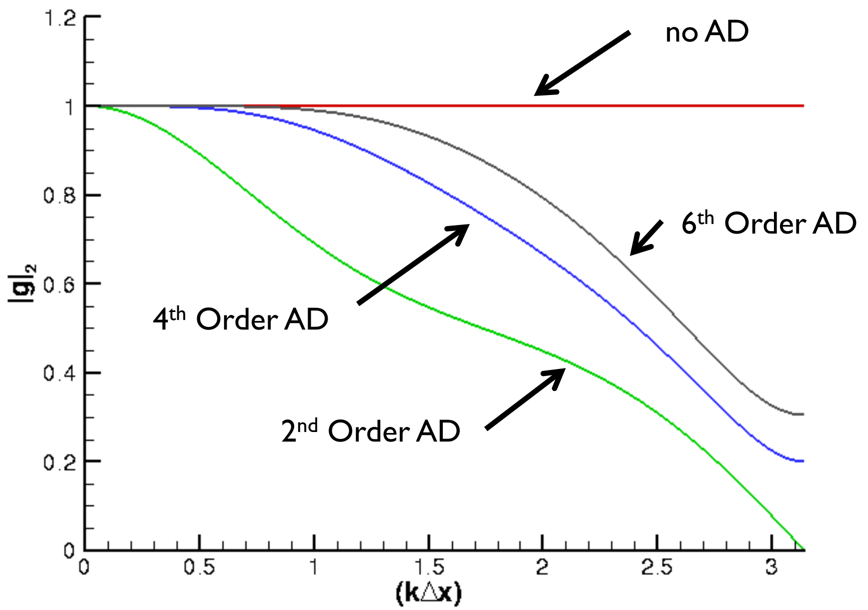
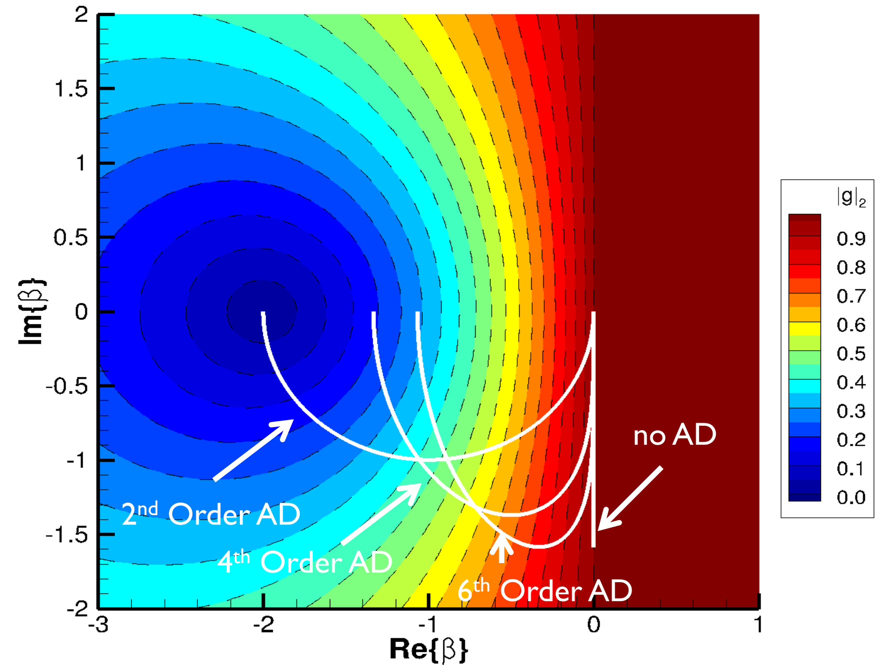
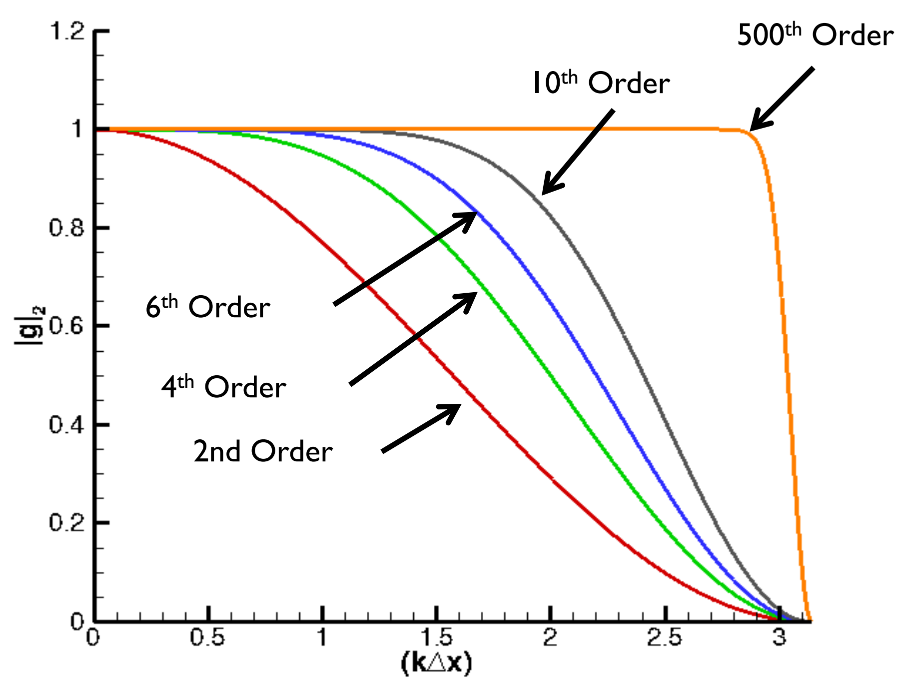
Artificial Dissipation: Growth Factor

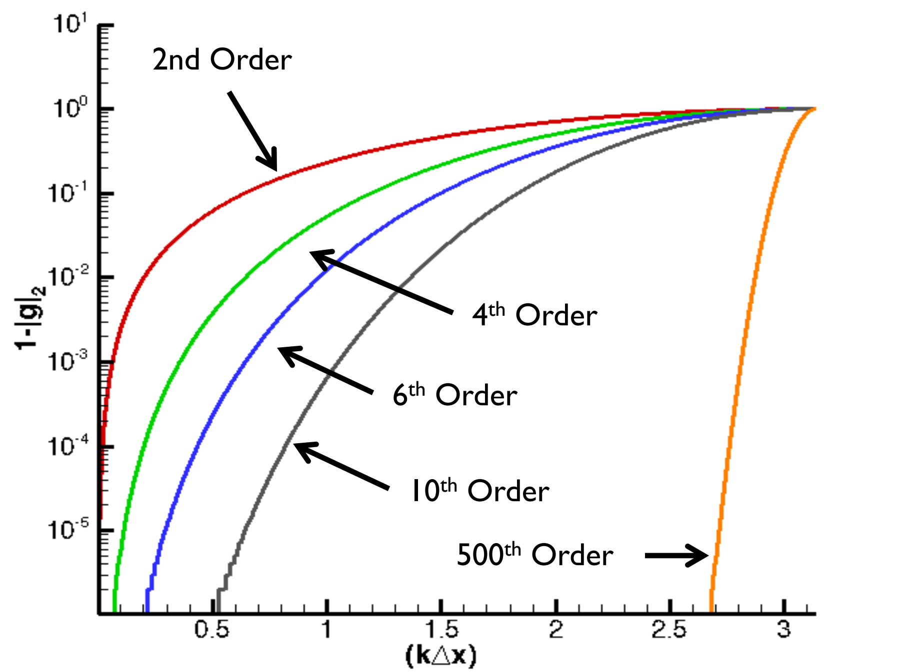




Explicit Filter: Growth Factor

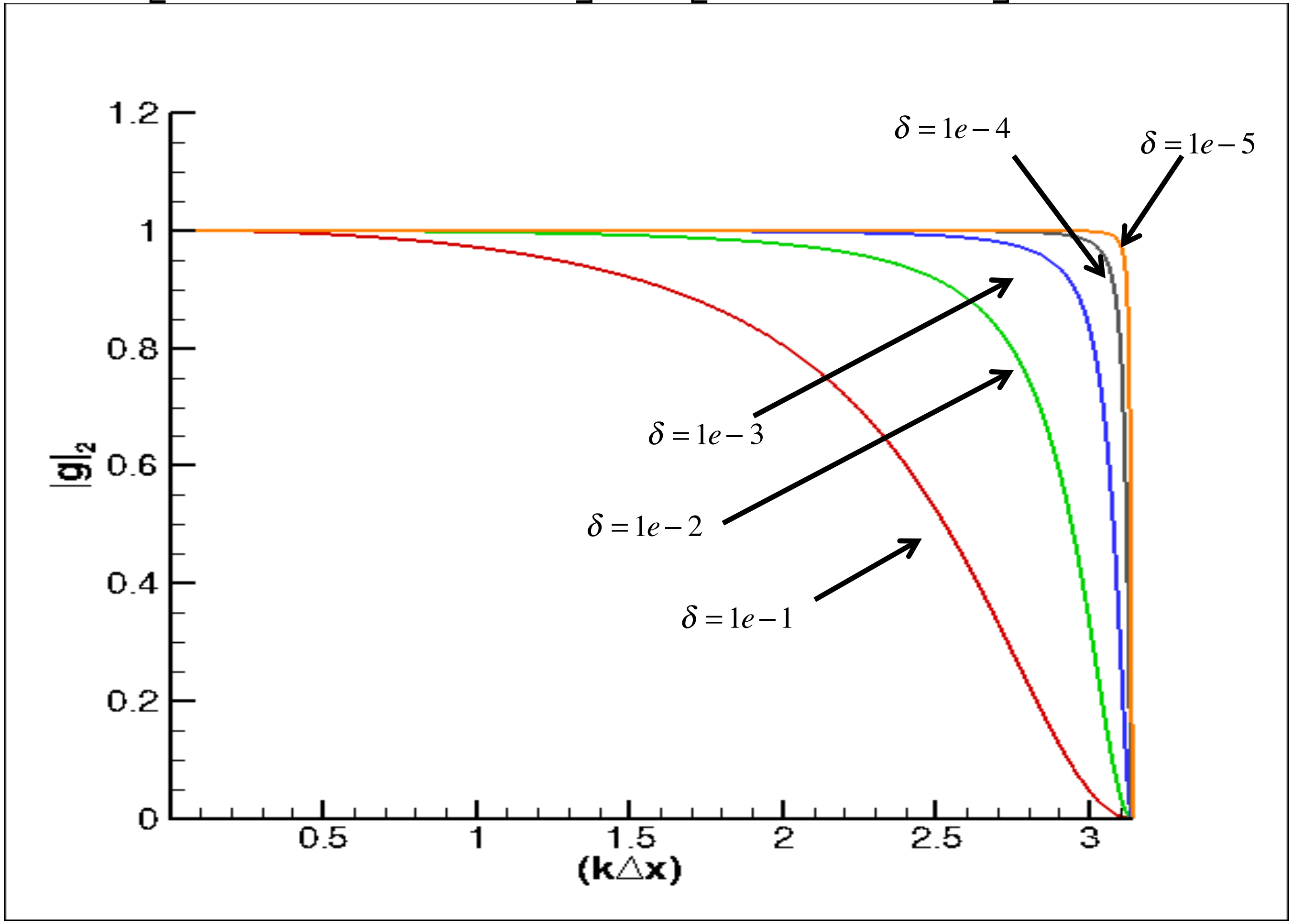
Shapiro Filter (1975) $$Q_i = \left[1 + S_m (\Delta x)^{2m} \frac{\partial^{2m}}{\partial x^{2m}}\right] Q_i^* \text{ with } S_m = \frac{(-1)^{m-1}}{2^{2m}}$$





2^{nd} Order Implicit Filter: Growth Factor

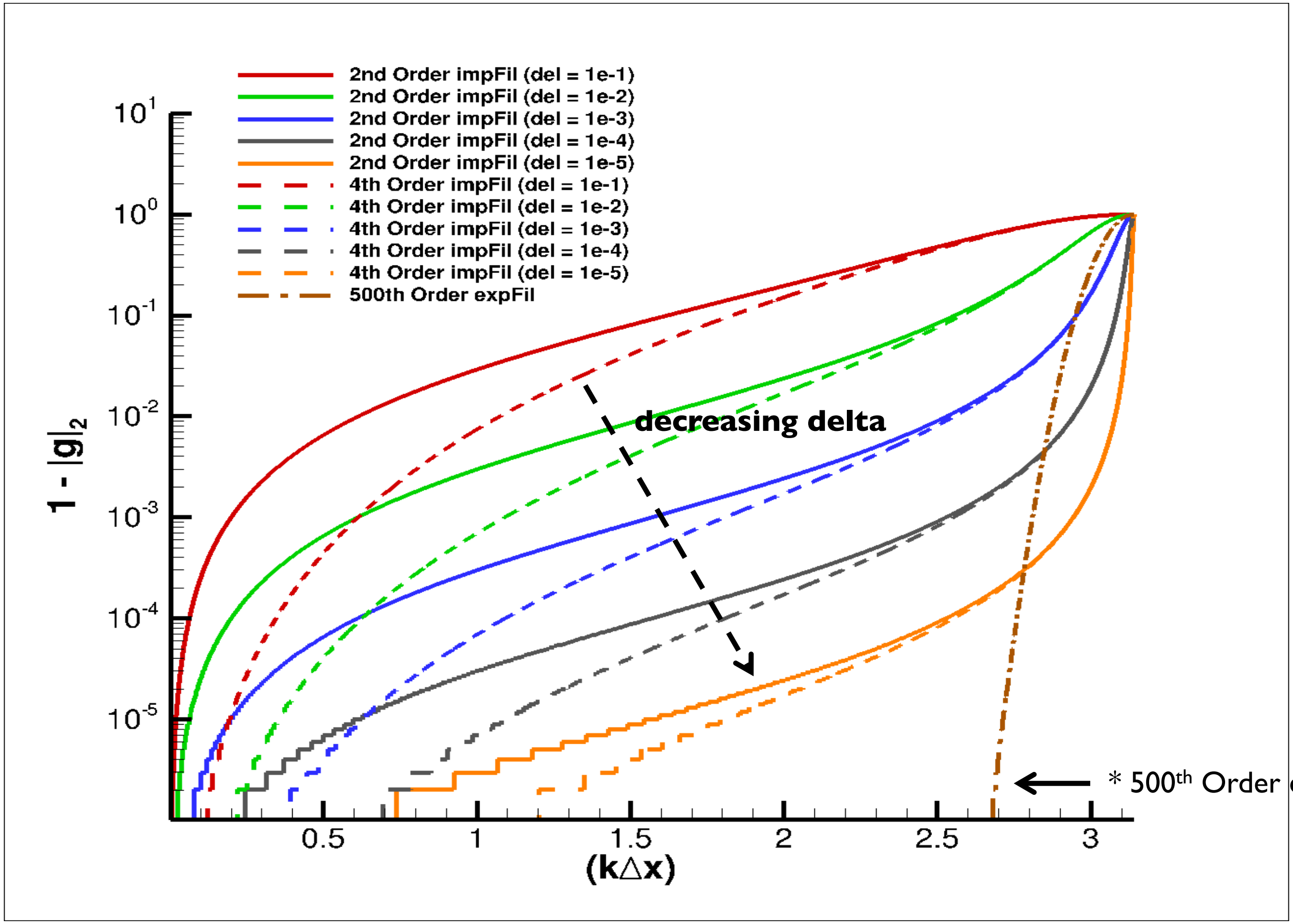
Long Filter (1971) $\left[1+(1-\delta)S(\Delta x)^2\frac{\partial^2}{\partial x^2}\right]Q_i=\left[1+S(\Delta x)^2\frac{\partial^2}{\partial x^2}\right]Q_i^*$ with $\delta\in\langle 0,1]$



2nd vs. 4th Order Implicit Filters: Growth Factor Error

4th order Lele Filter (1992)

$$\left[1+S(\Delta x)^2\frac{\partial^2}{\partial x^2}\right]Q_i=\left[1+S(\Delta x)^2\frac{\partial^2}{\partial x^2}+\left(\frac{-\delta}{4-8\delta}\right)S(\Delta x)^4\frac{\partial^4}{\partial x^4}\right]Q_i^* \quad \text{with } \delta\in\langle 0,1\rangle$$



Filtering as an Artificial Dissipation Scheme

$$Q_i^{n+1} = \left[1 + \frac{1}{4}(\Delta x)^2 \frac{\partial^2}{\partial x^2}\right] Q_i^*$$

$$= \left[1 + \frac{1}{4}(\Delta x)^2 \frac{\partial^2}{\partial x^2}\right]\left[Q_i^n - \Delta t(1-\theta)\frac{\partial E^n}{\partial x} + \Delta t\theta\frac{\partial E^*}{\partial x}\right] \text{ with } \theta \in [0,1]$$

$$\Downarrow$$

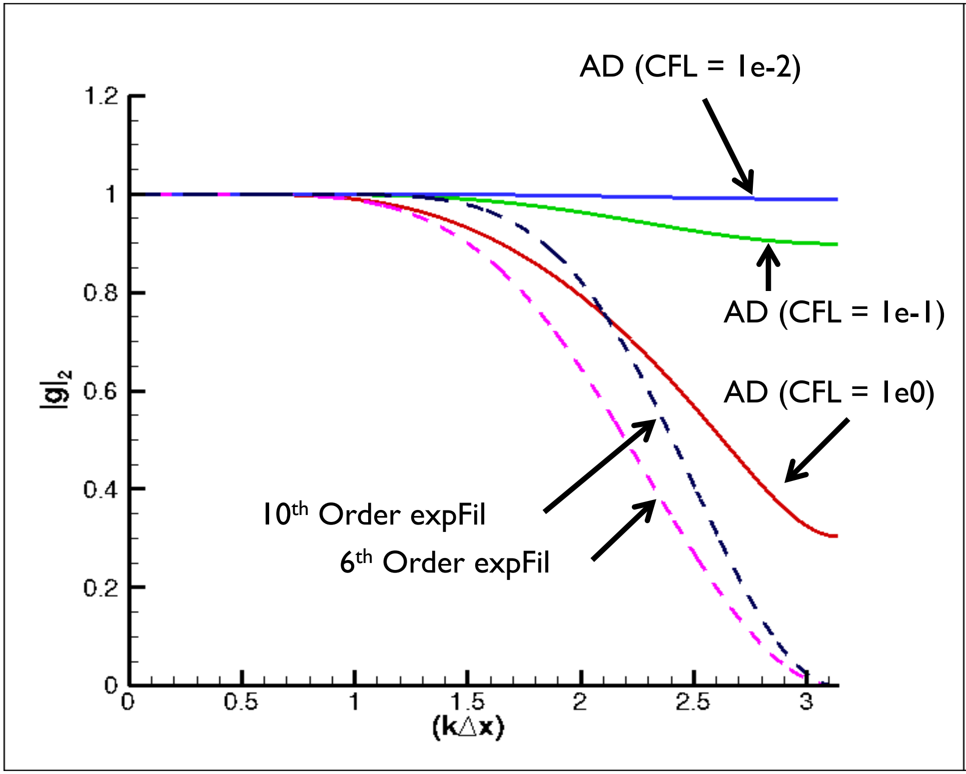
$$\frac{Q_i^{n+1} - Q_i^n}{\Delta t} + (1-\theta)\frac{\partial E^n}{\partial x} + (\theta)\frac{\partial E^*}{\partial x} = \frac{1}{4}\frac{(\Delta x)^2}{\Delta t}\frac{\partial^2 Q^n}{\partial x^2} - (1-\theta)\frac{1}{4}(\Delta x)^2\frac{\partial^3 E^n}{\partial x^3} - (\theta)\frac{1}{4}(\Delta x)^2\frac{\partial^3 E^*}{\partial x^3}$$

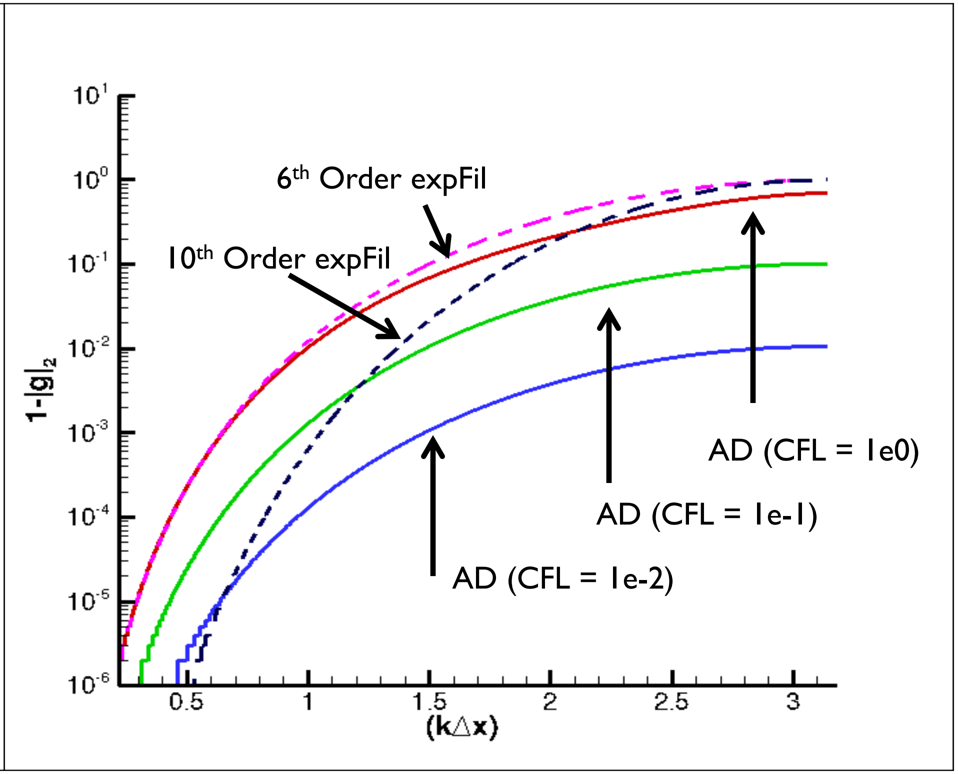
dispersive terms:
- restore phase of original scheme

dissipation term scales as $\varepsilon_2 \sim 1/CFL_{u+c}$
- increased damping w/ decreasing time-step

Effect of CFL

* AD shown is 6th order

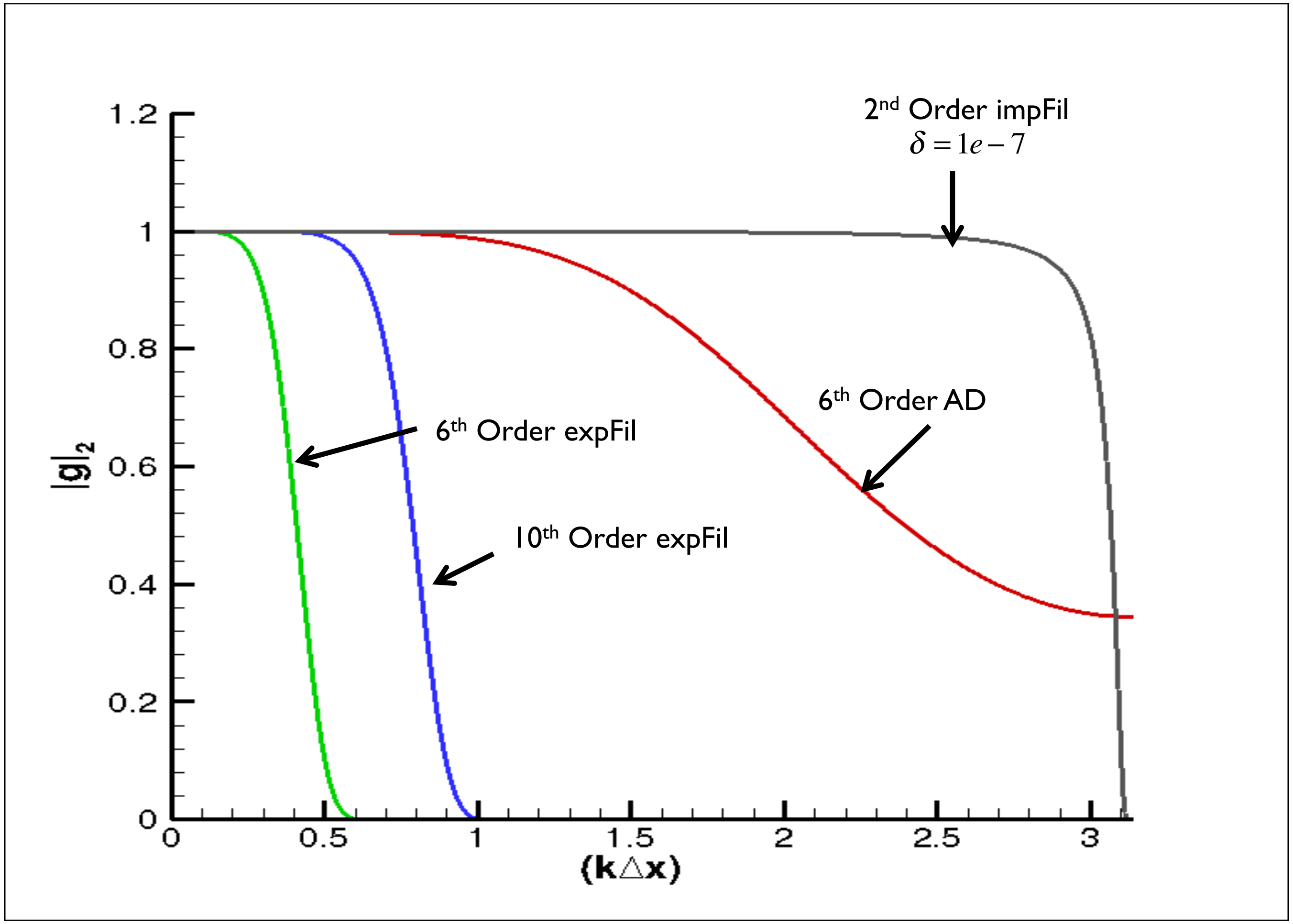




Cumulative Low CFL Damping

$CFL_{u+c} = 10^{-4}$

$\text{Nsteps} = 10^{4}$



Summary

- Filering is a form of artificial dissipation
  - damping behavior more predictable and tunable
- Explicit filters require very high order for low-pass response
  - overly dissipative for small time-steps
- Implicit filters can be efficiently designed for low-pass response
  - superior to artificial dissipation or explicit filters

Acknowledgments

guidance from advisors and collaborators:

- Dr. Venke Sankaran (Edwards AFRL)
- Professor Ann Karagozian (UCLA)
- Professor Charles Merkle (Purdue)

* support from Dr. Fariba Fahroo and Dr. Chiping Li (AFOSR)

THANK YOU

Back-Up Slides

Staggered Grid
Von Neumann Analysis

$$\frac{\partial Q}{\partial t} + \frac{\partial E}{\partial x} = 0$$ 1D Euler Eqns

Eigenvalues of the amplification matrix specify growth factor and phase errors.

$$Q^{n+1} = GQ^n$$

Staggered Grid Scheme/ Quasi-Linear Form

$$\Gamma_{ce}\left(\frac{\partial Q_{pT}}{\partial t} + \frac{\partial Q_u}{\partial t}\right)_i + \Gamma_m\left(\frac{\partial Q_{pT}}{\partial t} + \frac{\partial Q_u}{\partial t}\right)_{i+1/2} + A_{ce}\left(\frac{\partial Q_{pT}}{\partial x} + \frac{\partial Q_u}{\partial x}\right)_i + A_m\left(\frac{\partial Q_{pT}}{\partial x} + \frac{\partial Q_u}{\partial x}\right)_{i+1/2} = 0$$

$$Q_{pT} = \begin{pmatrix} p \\ 0 \\ T \end{pmatrix}$$

Continuity/Energy

Momentum

$$Q_u = \begin{pmatrix} 0 \\ u \\ 0 \end{pmatrix}$$

Growth Factor

$$||g_i||$$

Phase Error

$$\frac{\phi}{\phi_{exact}} = \frac{-\tan^{-1}\{Imag(g_i)/Re(g_i)\}}{CFL \times \beta}$$

Runge Kutta 4: von Neumann

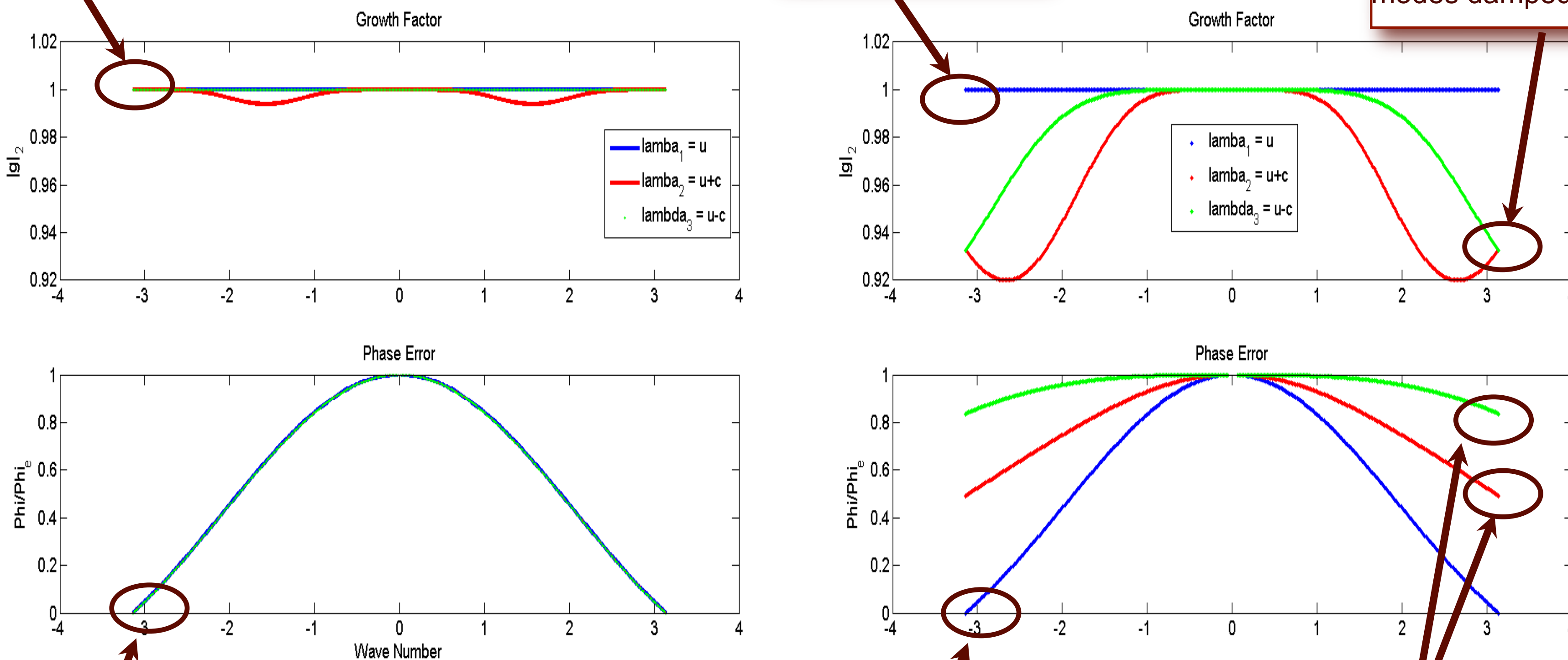
Collocated

Staggered

No damping of highest modes

No damping of PARTICLE WAVE's highest modes

Highest ACOUSTIC modes damped



No convection of highest modes

No convection of PARTICLE WAVE's highest modes

Slow convection of highest ACOUSTIC modes

Kinetic Energy Preservation (KEP)

- "in computations of turbulent flow fields, dissipative errors show up at the level of kinetic energy" (Mahesh 2004)
- Robust at inviscid limit (Re $\rightarrow \infty$)

Incompressible Flow:

$$u_i\left\{\frac{\partial u_i}{\partial t}+\frac{\partial u_i u_j}{\partial x_j}=\left(-\frac{\partial P}{\partial x_i}+\frac{\partial \tau_{ij}}{\partial x_j}\right)\right\} \xrightarrow{\frac{\partial u_j}{\partial x_j}=0} \frac{\partial}{\partial t}\left(\frac{1}{2}u_i^2\right)+\frac{\partial}{\partial x_j}\left(\frac{1}{2}u_i^2 u_j\right)=\left(-\frac{\partial u_i P}{\partial x_i}+u_i\frac{\partial \tau_{ij}}{\partial x_j}\right)$$

- $K = \frac{1}{2} u_i^2$ bounded and constant at inviscid limit
- KEP schemes satisfy secondary equation discretely
- Richtmeyer & Morton (1967)
- Arakawa (1966)

Compressible Flow:

$$\frac{-u_i^2}{2}\left\{\frac{\partial}{\partial t}\rho+\frac{\partial}{\partial x_j}\rho u_j\right\}+u_i\left\{\frac{\partial}{\partial t}\rho u_i+\frac{\partial}{\partial x_j}\rho u_i u_j+\frac{\partial}{\partial x_i}P-\frac{\partial}{\partial x_j}\tau_{ij}\right\}=0$$

$$\longrightarrow \frac{\partial}{\partial t}\left(\frac{1}{2}\rho u_i^2\right)+\frac{\partial}{\partial x_j}\left(\rho u_j\frac{u_i^2}{2}\right)=\left(-u_i\frac{\partial P}{\partial x_i}+u_i\frac{\partial \tau_{ij}}{\partial x_j}\right)$$

- Discrete analogue seeks:
  - Accurate transport of KE $\rightarrow$ accurate physical transfer of energy: $E = KE + U_{int}$

KEP: Applied to 1D Euler

(Collocated Grid)

- compare Crank-Nicolson (CN) with Fully KEP scheme (F-KEP)

$$\frac{(\rho\phi_k)_i^{n+1} - (\rho\phi_k)_i^n}{\Delta t} + \frac{1}{V_i}\sum_f (\phi)_f^m (\rho \mathrm{u}_j)_f^{n+1/2} \cdot S_i + \frac{1}{V_i}\sum_f \left(\frac{\partial p\upsilon_{k,j}}{\partial x_j}\right)_f^{n+1/2} \cdot S_i = 0$$

Subbareddy/Candler(2009)
Merkle (2013)

$$\phi^m = \frac{1}{2}(\phi^{n+1} + \phi^n)$$

(CN)

$$\phi^m = \frac{(\sqrt{\rho}\phi)^{n+1} + (\sqrt{\rho}\phi)^n}{(\sqrt{\rho})^{n+1} + (\sqrt{\rho})^n}$$

(F-KEP)

$$\phi = \begin{bmatrix} 1 \\ u \\ e \\ Y_k \end{bmatrix}$$

- discrete secondary equation satisfied to machine zero if KEP

$$\frac{(\rho\phi_k^2)_i^{n+1} - (\rho\phi_k^2)_i^n}{2\Delta t} + \frac{1}{V_i}\sum_f (\rho \mathrm{u}_j^{n+1/2})_f \left(\frac{\phi_k^2}{2}\right)_f^m \cdot S_{f,i} + \phi_{k,i}^m \frac{1}{V_i}\sum_f (p\upsilon_{k,j})^{n+1/2} \cdot S_{f,i} = RESIDUAL$$

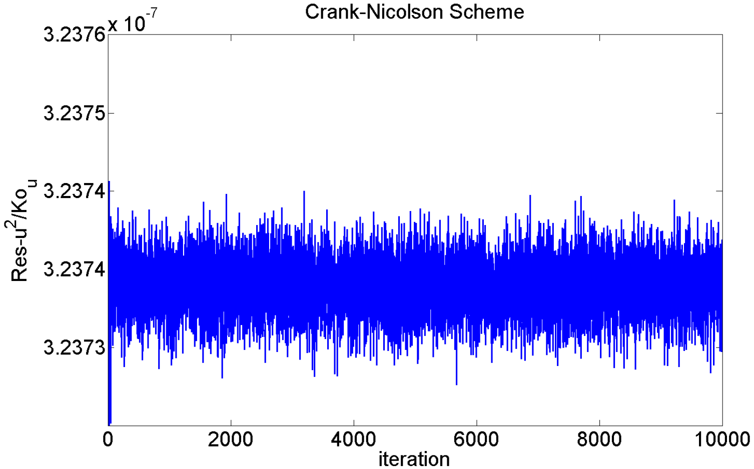
with $\left(\frac{\phi_k^2}{2}\right)_f^m = \frac{1}{2}\left(\frac{\phi_k}{2}\right)_i^m \left(\frac{\phi_k}{2}\right)_{nbr}^m$

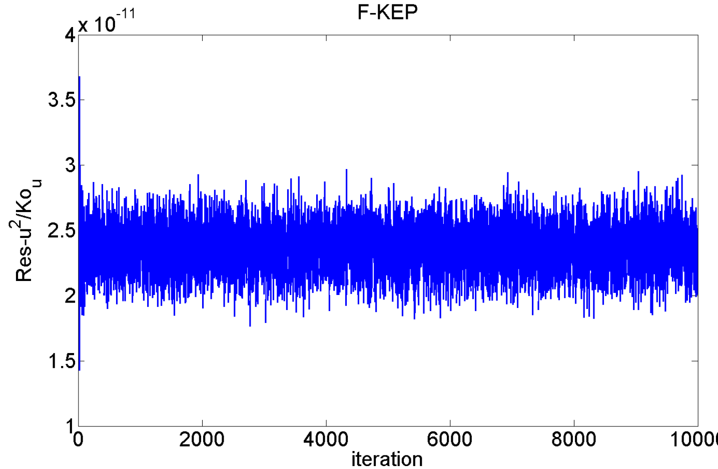
Evaluating KEP: u^2

Mach = 0.859

disturb = 0.01%

- F-KEP always secondary conservative
- CN is KEP for low compressibility effects





disturb = 1%